



**YOGI VEMANA UNIVERSITY**  
Vemanapuram, KADAPA-516003, Andhra Pradesh, INDIA  
<http://www.yogivemanauniversity.ac.in>

**DEPARTMENT OF CHEMISTRY**  
**CURRICULUM-MSc ORGANIC CHEMISTRY**

**M.Sc. Previous**

S. No.	Paper Number	Paper's Title	Contact Hrs per Week		Uni.Exam Duration (Hrs)		Distribution of Marks					
			L	P	T	P	IE	TE	PE	R	V	TOTAL
<b>III-SEMESTER</b>			L	P	T	P	IE	TE	PE	R	V	TOTAL
1	15031	Inorganic Chemistry	4	-	3	-	25	75	-	-	-	100
2	15032	Organic Chemistry	4	-	3	-	25	75	-	-	-	100
3	15033	Physical Chemistry	4	-	3	-	25	75	-	-	-	100
4	15034	General Chemistry –I	4	-	3	-	25	75	-	-	-	100
5	15031P	<i>Inorganic chemistry Practicals</i>	-	9	-	3	-	-	75	10	15	100
6	35032P	<i>Organic chemistry Practicals-I</i>	-	9	-	3	-	-	75	10	15	100
7		Seminar	2	-	-	-	-	-	-	-	-	-
<b>Total Hours/Week</b>			<b>18</b>	<b>18</b>	-	-	<b>Total Marks</b>					<b>600</b>

S. No.	Paper Number	Paper's Title	Contact Hrs per Week		Uni.Exam Duration (Hrs)		Distribution of Marks					
			L	P	T	P	IE	TE	PE	R	V	TOTAL
<b>IV-SEMESTER</b>			L	P	T	P	IE	TE	PE	R	V	TOTAL
1	25031	Inorganic Chemistry	4	-	3	-	25	75	-	-	-	100
2	25032	Organic Chemistry	4	-	3	-	25	75	-	-	-	100
3	25033	Physical Chemistry	4	-	3	-	25	75	-	-	-	100
4	25034	General Chemistry –II	4	-	3	-	25	75	-	-	-	100
5	25031P	<i>Organic chemistry Practicals-II</i>	-	9	-	3	-	-	75	10	15	100
6	25032P	<i>Physical chemistry Practicals</i>	-	9	-	3	-	-	75	10	15	100
7		Seminar	2	-	-	-	-	-	-	-	-	-
<b>Total Hours/Week</b>			<b>18</b>	<b>18</b>	-	-	<b>Total Marks</b>					<b>600</b>

**L- Lecture    P- Practical    T- Theory    IE- Internal Examination**

**TE- Theory Examination    PE- Practical Examination    R-Record    V-Vivo Voce**

**M.Sc. Final**

S. No.	Paper Number	Paper's Title	Contact Hrs per Week		Uni.Exam Duration (Hrs)		Distribution of Marks					
			L	P	T	P	IE	TE	PE	R	V	TOTAL
<b>III-SEMESTER</b>			L	P	T	P	IE	TE	PE	R	V	TOTAL
1	35031	Inorganic Chemistry	4	-	3	-	25	75	-	-	-	100
2	35032	Organic Chemistry	4	-	3	-	25	75	-	-	-	100
3	35033	Physical Chemistry	4	-	3	-	25	75	-	-	-	100
4	35034	Spectroscopy and its Applications	4	-	3	-	25	75	-	-	-	100
5	35031P	<i>Chromatographic Separation and Isolation &amp; Identification of Natural Products</i>	-	9	-	3	-	-	75	10	15	100
6	35032P	<i>Estimations</i>	-	9	-	3	-	-	75	10	15	100
7		Seminar	2	-	-	-	-	-	-	-	-	-
		<b>Total Hours/Week</b>	<b>18</b>	<b>18</b>	-	-	<b>Total Marks</b>					<b>600</b>

S. No.	Paper Number	Paper's Title	Contact Hrs per Week		Uni.Exam Duration (Hrs)		Distribution of Marks					
			L	P	T	P	IE	TE	PE	R	V	TOTAL
<b>IV-SEMESTER</b>			L	P	T	P	IE	TE	PE	R	V	TOTAL
1	45031	Reactions and Reagents in Organic Synthesis	4	-	3	-	25	75	-	-	-	100
2	45032	Synthetic Strategies and Drug Design	4	-	3	-	25	75	-	-	-	100
3	45033	Heterocyclic Chemistry and Biomolecules	4	-	3	-	25	75	-	-	-	100
4	45034	Chemistry of Natural Products	4	-	3	-	25	75	-	-	-	100
5	45031P	<i>Multistep Synthesis of Organic Compounds</i>	-	9	-	3	-	-	75	10	15	100
6	45032P	<i>Spectral Identification of Organic Compounds</i>	-	9	-	3	-	-	75	10	15	100
7		Seminar	2	-	-	-	-	-	-	-	-	-
		<b>Total Hours/Week</b>	<b>18</b>	<b>18</b>	-	-	<b>Total Marks</b>					<b>600</b>

L- Lecture    P- Practical    T- Theory    IE- Internal Examination  
 TE- Theory Examination    PE- Practical Examination    R-Record    V-Vivo Voce

Note: Open elective -1 and 2 will be offered to the students of other departments in the II<sup>nd</sup> and III<sup>rd</sup> semesters, respectively

**FIRST SEMESTER**  
**15031: INORGANIC CHEMISTRY**

**UNIT-I: Metal – Ligand Bonding Theories**

**UNIT-II: Metal-ligand equilibria in solution and theory of HSAB**

**UNIT-III: Reaction mechanisms of complexes**

**UNIT-IV: Carbonyl and Nitrosyl Complexes, and Metal Atom Clusters**

**UNIT-I: Metal – Ligand Bonding Theories**

**15 Hrs**

Crystal Field Theory (CFT) for bonding in transition metal complexes, crystal field splitting of 'd'-orbitals in octahedral, tetrahedral, tetragonal and square planar fields. Crystal Field Stabilization Energy (CFSE) and its calculation in six and four coordinated complexes, Spectrochemical series with reference to ligands and metal ions. Factors affecting the magnitude of  $\Delta_o$  in octahedral complexes, Jahn-Teller effect and its consequences. Shortcomings of CFT; Covalency: Evidence for covalency, Nephelauxetic effect; Molecular orbital theory: Concept of Ligand Groups Orbitals (LGOs), MO diagrams for octahedral, tetrahedral and square planar complexes, MO treatment of  $\pi$ -bonds.

**UNIT-II: Metal-ligand equilibria in solution and theory of HSAB**

**15 Hrs**

**(A) Metal-ligand equilibria in solution**

Stepwise and overall formation constants and their interrelationship, Trends in stepwise formation constants, Factors affecting the stability of metal complexes, Chelate effect, Determination of binary formation constants by  $p^H$ -metry and spectrophotometric methods.

**(B) Theory of HSAB**

Hard and soft acids and bases, Classification, Acid-base strength and hardness, Symbiosis, Electronegativity and hardness, Application of HSAB: Biological functions and toxicology of metals, and medicinal applications.

**UNIT-III: Reaction mechanisms of complexes**

**15 Hrs**

Reactivity of metal complexes, Inert and labile complexes, Kinetics and mechanisms of substitution reactions, Kinetics of substitution reactions in octahedral complexes, Acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reactions, Substitution reactions in square planar complexes, Trans effect, Mechanism of trans effect, Electron transfer reactions, Inner sphere and outer sphere mechanisms, Marcus theory.

**UNIT-IV: Carbonyl and Nitrosyl Complexes, and Metal Atom Clusters**

**15 Hrs**

**(A) Metal Carbonyl and nitrosyl complexes**

Metal carbonyls: Preparation of metal carbonyls of Mn, Fe, Co and Ni, Bonding in carbonyls, EAN and 18-electron rule in carbonyls,  $\pi$ -Bonding in carbonyls, Terminal and bridging carbonyls, Measurement of  $\sigma$  -  $\pi$  bond strength in carbonyls, Structures of mononuclear, binuclear, trinuclear and tetranuclear carbonyls; Metal nitrosyls: Chemistry of linear and bent nitrosyls, Nitrosyls as  $NO^+$  and  $NO^-$  donors, Analytical uses of nitrosyl complexes.

**(B) Metal atom clusters**

Cage structures, Higher boranes, Carboranes, Metal-metal bonds in carbonyl cluster, LNCCs and HNCCs, Isoelectronic and isolobal relationships, Hetero atom in metal atom clusters, Electron counting schemes for HNCCs,

HNCCs of Fe, Co, Ni, Ru, Rh, Pd, Os, Ir and Pt, Lower halide and chalcogenide clusters, Triangular clusters, Solid state extended arrays.

**Books suggested:**

1. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, M. Bochmann and R. N. Grimes, 5<sup>th</sup> Ed. (John Wiley & Sons Inc.).
2. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4<sup>th</sup> Ed. (Prentice Hall).
3. Inorganic Chemistry: G. Wulfsberg (University Science Books).
4. Introduction to Ligand Fields, B. N. Figgis (Krieger Pub Co.).
5. Concise Inorganic Chemistry, J. D. Lee, 5<sup>th</sup> Ed. (Wiley-Blackwell).
6. Modern Inorganic Chemistry, W. L. Jolly, 2<sup>nd</sup> Ed. (McGraw-Hill).
7. Coordination Compounds, S. F. Kettle (Springer).

## 15032: ORGANIC CHEMISTRY

### UNIT-I: Nature of bonding in organic molecules and aromaticity

### UNIT-II: Reaction Mechanism and Reactive intermediates

### UNIT-III: Nucleophilic Substitution reactions

### UNIT-IV: Stereo Chemistry

### UNIT-I: Nature of bonding in organic molecules and aromaticity

15Hrs

#### (A) Electronic Effects

Inductive effect, mesomeric effect (Resonance), hyperconjugation, steric effect, tautomerism, acidity and basicity of organic molecules

#### (B) Criteria of Aromaticity

The Energy Criterion for Aromaticity, Structural Criteria for Aromaticity, Electronic Criteria for Aromaticity, Relationship among the Energetic, Structural, and Electronic Criteria of Aromaticity, Huckel's rule and MO Theory, aromaticity in benzenoid, non-benzenoid compounds, Aromaticity in Charged Ring Fused-Ring Systems, Heteroaromatic Systems, Annulenes: Cyclobutadiene, Benzene, 1,3,5,7-Cyclooctatetraene, [10] Annulenes-1,3,5,7,9-Cyclodecapentaene Isomers, [12], [14], [16] and [18] annulenes, azulenes, fulvenes, fullerenes, ferrocene, anti-aromaticity, homo-aromaticity.

### UNIT-II: Reaction Mechanism and Reactive intermediates

15Hrs

#### (A) Determination of reaction mechanism

Type of reactions with mechanism, Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Potential energy diagrams, Transition states, Intermediates, methods of determining mechanisms, Isotope effects, Linear free energy relationships and their applications.

#### (B) Reactive intermediates

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes

### UNIT-III: Nucleophilic Substitution reactions

15Hrs

#### (A) Aliphatic nucleophilic substitutions

$S_N^1$  and  $S_N^2$  reactions: mechanism, energy profile diagram, stereochemistry and evidence in favour of the mechanism, SET and Border line (mixed  $S_N^1$  and  $S_N^2$ ) mechanisms, Neighbouring group participation, Anchimeric assistance, Nonclassical carbocations, Phenonium ions, Norbornyl system, Common carbocation rearrangements- primary, secondary and tertiary,  $S_N^1$  and  $S_N^1$  mechanisms, Tetrahedral mechanism, Nucleophilic substitution at an allylic and aliphatic trigonal carbon. Factors influencing on nucleophilic substitution reactions: the structure of the substrate, the solvent, the nucleophile and the leaving group.

#### (B) Aromatic nucleophilic substitution

$S_N^1$ ,  $S_N$  Ar (energy profile diagram and evidence for the mechanism), and benzyne mechanisms, Von Richter, Sommelet-Hauser and Smiles rearrangements.

### UNIT-IV: Stereo Chemistry

15Hrs

#### (A) Molecular representation of organic molecules

Wedge, Fischer, Newman and Sawhorse formula, their description, inter conversion.

**(B) Molecular Symmetry and Chirality**

Symmetry elements, Definition and classification of Stereoisomers, Enantiomer, Diastereomer, Invertomer, Homomer, Epimer, Anomer, Configuration and Conformation

Configurational nomenclature: D,L and R, S nomenclature, Molecules with a single chiral center: Tetra and Tri coordinate chiral center, Molecules with two or more chiral centers: constitutionally unsymmetrical and symmetrical molecules.

**(C) Geometrical Isomerism**

Cis-trans, E, Z- and Syn & anti nomenclature, Methods of determining configuration of Geometrical isomers using physical, spectral and chemical methods, Stability, Cis-trans inter conversion.

**(D) Stereoisomerism in molecules without chiral Center: Axial chirality**

Allenes, Alkylidenecycloalkanes, spiranes, nomenclature, Atropisomerism: biphenyl derivatives, nomenclature, **Planar chirality:** Ansa compounds, paracyclophanes, trans-cyclooctene, Helicity

**Books Suggested:**

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6<sup>th</sup> Ed. (John Wiley & Sons).
2. Organic Chemistry, Paula Yurkanis Bruice, 4<sup>th</sup> Ed. (Printice Hall)
3. Organic chemistry-Clayden J. (Oxford)
4. Organic Chemsitry, Wade, L.G. Jr. 5<sup>th</sup> Ed. (Pearson)
5. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2<sup>nd</sup> Ed. (Pearson)
6. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.).
7. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6<sup>th</sup> Ed., (Longman).
8. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2<sup>nd</sup> Ed. (New Age International).
9. Organic Chemistry, R. T. Morrison and R. N. Boyd (Prentice-Hall)
10. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
11. Stereochemistry to Organic Compounds, D. Nasipuri, 2<sup>nd</sup> Ed. (New Age International).
12. Stereochemistry, P.S. Kalsi, 5<sup>th</sup> Ed. (New Age International).
13. Organic Chemistry Structure and Reactivity, Ege Seyhan, 3<sup>rd</sup> Ed. (AITBS)

## 15033: PHYSICAL CHEMISTRY

### UNIT – I : Quantum Chemistry-I

### UNIT – II: Chemical Dynamics-I

### UNIT – III: Thermodynamics-I

### UNIT – IV: Electrochemistry-I

### UNIT – I : Quantum Chemistry-I

15 Hrs

#### (A) Introduction to Exact Quantum Mechanical Results

Operator algebra, Eigen values and Eigen functions, Operators for momentum and energy, Linear combination of Eigen functions of an operator. The Schrodinger wave equation and the postulates of Quantum Mechanics, Discussion of solutions of the Schrodinger equation to some model systems, viz., particle in a box, harmonic oscillator, rigid rotor, hydrogen atom. Application of the spectra of conjugated molecules.

#### (B) Approximate Methods

The Variation Theorem, Linear variation Principle, Perturbation Theory (first Order and non-degenerate), Application of Variation Method and Perturbation theory to the Helium atom,

### UNIT – II: Chemical Dynamics-I

15 Hrs

#### (A) Theories of reaction rates

Collision theory, steric factor. Theory of Absolute Reaction Rates-Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of reaction rates, Arrhenius Equation

#### (B) Unimolecular reactions

Lindemann, Lindemann-Hinshelwood, and RRKM theories. Termolecular reactions. Complex reactions-Rate expressions for opposing, parallel and consecutive reaction (all first order type)

#### (C) Chain reactions

Dynamic chain, hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane, photochemical reactions-  $\text{H}_2\text{-Br}_2$ ,  $\text{H}_2\text{-Cl}_2$  reactions, Autocatalysis,  $\text{H}_2\text{-O}_2$  reaction, explosion limits, rate expressions for chain reaction.

### UNIT – III: Thermodynamics-I

15 Hrs

#### (A) Brief review of Thermodynamic concepts

Enthalpy, entropy, free energy. Concept of Entropy - Entropy as a state function - Entropy change in reversible process and irreversible process - Temperature -Entropy diagrams - Entropy change and Phase change - Entropy of mixing -Entropy and disorder.

#### (B) Classical & Statistical thermodynamics

Partial molar properties: their significance and determination of partial molar volume, fugacity and its determination. Concept of distribution, thermodynamic probability and most probable Distribution, Ensemble averaging, Postulates of ensemble averaging, canonical, grand canonical and micro-canonical ensembles, partition functions, translational, rotational, vibrational and electronic partition functions, Gibbs-Duhem equation, calculation of thermodynamic properties in terms of partition functions, Heat capacity, chemical equilibria and equilibrium constant in terms of partition functions, Entropy of monatomic gases (Sackur-Tetrad equation)

**(A) Strong Electrolytes**

Effect of dilution on equivalent conductance-Inter ionic attraction, Debye-Huckel-Onsager treatment, derivation of Debye-Huckel-Onsager equation, Verification and limitation of Onsager equation, Bjerrum treatment of electrolytes, Debye-Falkenhagen and Wien effects.

**(B) Activity and activity coefficients**

Relation between different types of activity coefficients, Determination of mean ionic activity coefficients by solubility and EMF methods, Debye-Huckel Limiting law and its verification (qualitative).

**(C) Reversible electrochemical cells**

Chemical cells and concentration cells-Types of reversible electrodes-Electrode potentials. Reactions in reversible cells - Nernst equation- thermodynamic and kinetic derivation-Concentration cells with and without transference. Liquid junction potential and its determination.

**Books suggested**

1. Physical Chemistry, P. W. Atkins (ELBS)
2. Introduction to quantum Chemistry, A. K. Chandra (Tata McGraw Hill)
3. Quantum Chemistry, Ira N. Levine (Prentice Hall)
4. Atomic Structure and chemical bond, Manas Chandra.
5. Chemical Kinetics, K.J.Laidler (McGraw Hill)
6. Kinetics and Mechanism of chemical Transformations, J. Rajaraman and J. Kuriacose (McMilan)
7. Thermodynamics for Chemists, S. Glasstone
8. Chemical Thermodynamics, I. M. Klotz
9. Statistical Thermodynamics, M. Dole
10. Modern Electrochemistry, vol. I & II, J. O. M. Bockris and A. K. N. Reddy (Plenum)
11. An Introduction to Electrochemistry (3<sup>rd</sup> ed.), S. Glasstone (A ffiliated East-West)



## 15034: GENERAL CHEMISTRY – I

### UNIT-I: Symmetry and Group Theory

### UNIT-II: Errors and Statistics

### UNIT-III: Microwave Spectroscopy, Infrared Spectroscopy, Raman Spectroscopy

### UNIT-IV: Electron Spin Resonance (ESR) and Mössbauer Spectroscopy

#### UNIT-I: Symmetry and Group Theory

15 Hrs

Symmetry Elements and Symmetry operation, Definitions of a group, sub-group, Relation between orders of a finite group and its sub-group, Conjugacy Relation and classes-point symmetry group, Schonflies symbols, Representation of groups by matrices (representation for  $C_{n^9}$ ,  $C_{n^9}$ ,  $D_{nh^9}$  etc. groups to be worked out explicitly), character of a representation. The great orthogonality theorem (without proof), Character tables and their use in spectroscopy.

#### UNIT-II: Errors and Statistics

15 Hrs

Classification of errors; accuracy; precision; minimization of systematic errors; mean and median values; absolute error; relative error; mean deviation and relative mean deviation; standard deviation and relative standard deviation; variance; range; confidence interval; comparison of results: F-test and student's t-test (i. comparison of mean and true value, ii. comparison of two means and iii. comparison of more than two means - ANOVA); Gaussian distribution of random errors; correlation and regression; linear-least-square fitting; significant figures and rules of significant figures.

#### UNIT-III: Microwave Spectroscopy, Infrared Spectroscopy, Raman Spectroscopy

15Hrs

##### (A) Microwave Spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, stark effect.

##### (B) Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero-point energy, force constant, bond strengths, anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, PQR branches, Vibrations of simple polyatomic molecules ( $CO_2$ ,  $H_2O$  etc.), Selection rules, exclusion principle.

##### (C) Raman Spectroscopy

Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational – rotational Raman spectra, selection rules.

#### UNIT-IV: Electron Spin Resonance (ESR) and Mössbauer Spectroscopy

15 Hrs

**(A) Electron Spin Resonance Spectroscopy:** Introduction, Principle, instrumentation, selection rules, g-factor and its significance, hyperfine and super hyperfine coupling, Zero-field splitting (ZFS), Kramer's degeneracy. Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bissalicylaldimine, Bis-acetylacetonatovanadyl and hexachloroiridium(IV) complexes.

**(B) Mössbauer Spectroscopy:** Basic principles, Isomer shift, Quadrupole shift and spectrum display, Applications: Bonding and structures of  $Fe^{2+}$  and  $Fe^{3+}$  compounds including those of intermediate spin and  $Sn^{2+}$  and  $Sn^{4+}$  compounds, Nature of metal-ligand bond, Coordination number, Unequivalent mössbauer atoms.

#### Books Suggested

1. Symmetry and Spectroscopy molecules –K. Veera Reddy, New Age Publications, New Delhi.
2. Chemical Applications of Group Theory by Bhattacharya
3. Vogel's Text Book of Quantitative Chemical Analysis, J. Vogel, R. C. Denney, J. D. Barnes and M. J. Thomas, 4<sup>th</sup> & 6<sup>th</sup> Ed.(Pearson Education Asia).
4. Analytical Chemistry by Robert Drills
5. Quantitative Analysis by R. A. Day and A. L. Underwood.
6. Analytical Chemistry, G. D. Christian
7. Instrumental Methods of Analysis, H. W. Willard, L. L. Merritt and J. A. Dean (Affiliated East-West)
8. Principles of Instrumental Analysis, D. A. Skoog and D. M. West (Holt, Rinehart and Wilson)
9. Physical Methods in Chemistry, R. S. Drago (Saunders).
10. Introduction to molecular Spectroscopy, G. M. Barrow (McGraw Hill)
11. Basic principles of Spectroscopy, R. Chang (Mc Graw Hill)

## Laboratory Course-200 MARKS

### I – SEMESTER

#### 15031P: INORGANIC CHEMISTRY PRACTICALS

1. Semi-micro qualitative analysis of a mixture containing four cations including rare elements:  
(Rare elements: Te, W, Se, Mo, Zr, Ce, Th, V, and U).
2. Preparation and purification of inorganic complexes
  - a) *tris*(thiourea)zinc(II)sulphate
  - b) *cis*-potassium *tris*(oxalato)ferrate(III)trihydrate
  - c) *tris*(acetylacetonato)manganese(III)
  - d) hexaminenickel(II)chloride
  - e) *bis*(acetylacetonato)copper(II)

#### 15032-P: ORGANIC CHEMISTRY PRACTICALS

Preparation, recrystallization, and determination of melting point & yield of the following compounds:

- (i) Aspirin, (ii) Nerolin, (iii) Chalcone, (iv) *p*-nitro acetanilide, (v) *p*-nitro acetanilide, (vi) *m*-dinitrobenzene, (vii) phthalimide, (viii) hippuric acid, and (ix) Diels-Alder adduct.

#### Books Suggested

1. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, 4<sup>th</sup> & 6<sup>th</sup> Ed. (Pearson Education Asia).
2. Vogel's Text Book of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, 5 Ed. (Longman Scientific & Technical)

**SECOND SEMESTER**  
**25031: INORGANIC CHEMISTRY**

**UNIT-I: Organometallic Chemistry**

**UNIT – II: Transition Metal  $\pi$ -Complexes**

**UNIT – III: Electronic Spectra of Complexes**

**UNIT – IV: Magnetic Properties of Transition Metal Complexes**

**UNIT-I: Organometallic Chemistry**

**15 Hrs**

**(A) Organo-metallic Reagents in Synthesis:** Stoichiometric reactions in catalysis, Homogeneous catalytic hydrogenation, Hydroformylation (oxo reaction), Isomerisation, Zeigler-Natta polymerization of olefins, Oxopalladation reactions, Activation of small molecules by coordination.

**(B) Fluxional Organometallic Compounds:** Fluxionality and dynamic equilibria in compounds such as  $\eta^2$ -olefin,  $\eta^3$ -allyl and dienyl complexes.

**UNIT – II: Transition Metal  $\pi$ -Complexes**

**15 Hrs**

Transition metal  $\pi$ -complexes with unsaturated organic molecules such as alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, General methods of preparation, Properties, Nature of bonding and structural features, Important reactions relating to nucleophilic and electrophilic attack on ligands.

**UNIT – III: Electronic Spectra of Complexes**

**15 Hrs**

Free Ion Terms and Energy Levels: Configurations, Terms, States and Microstates. Calculation of Microstates for  $p^2$  and  $d^2$  configuration, L-S (Russell-Saunders) Coupling Schemes, J-J Coupling scheme, derivation of terms for  $p^2$  and  $d^2$  configuration. Hole Formulation, Energy ordering of terms (Hund's Rules), Selection rules: Laporte orbital selection rule, spin selection rules. Splitting of energy levels and spectroscopic states, Orgel diagrams of  $d^1$  to  $d^9$  metal complexes. Interpretation of electronic spectra of aquo complexes of Ti(III), V(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II). Calculation of interelectronic and spectra parameters for  $d^8$  metal complexes. Tanabe-Sugano diagrams for  $d^2$  and  $d^6$  octahedral complexes. Charge transfer ( $L \rightarrow M$  and  $M \rightarrow L$ ) spectra of metal complexes.

**UNIT – IV: Magnetic Properties of Transition Metal Complexes**

**15 Hrs**

Diamagnetism, Paramagnetism, Orbital and spin contributions, Spin-orbit coupling, Hund's third rule and energies of J levels, Curie law and Curie-Weiss law, Ferromagnetism and antiferromagnetism, Temperature independent magnetism, Magnetic susceptibility and determination of magnetic susceptibility by Gouy method, Paramagnetism and crystalline fields –  $Ti^{3+}$ ,  $V^{3+}$ ,  $VO^{2+}$ ,  $Cr^{3+}$ ,  $Mn^{2+}$ ,  $Fe^{3+}$ ,  $Co^{2+}$ ,  $Ni^{2+}$  and  $Cu^{2+}$ , Magnetic exchange in copper acetate and other dimers.

**Books Suggested:**

1. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, M. Bochmann and R. N. Grimes, 5<sup>th</sup> Ed. (John Wiley & Sons Inc.).
2. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4<sup>th</sup> Ed. (Prentice Hall).
3. Inorganic Chemistry: G. Wulfsberg (University Science Books).
4. Introduction to Ligand Fields, B. N. Figgis (Krieger Pub Co.).
5. Concise Inorganic Chemistry, J. D. Lee, 5<sup>th</sup> Ed. (Wiley-Blackwell).
6. Modern Inorganic Chemistry, W. L. Jolly, 2<sup>nd</sup> Ed. (McGraw-Hill).
7. Coordination Compounds, S. F. Kettle (Springer).
8. Magnetochemistry, R. L. Carlin (Springer-Verlag New York).
9. Elements of Magnetochemistry R. L. Dutta and A. Syamal, 2<sup>nd</sup> Ed. (Affiliated East-West Press Pvt. Ltd).
10. The Organometallic Chemistry of the Transition Metals, R. H. Crabtree, 3<sup>rd</sup> and 4<sup>th</sup> Ed. (Wiley Interscience).
11. Organometallic Chemistry: A Unified Approach, R. C. Mehrotra and A. Singh, 2<sup>nd</sup> Ed. (New Age International).
12. Principles of Organometallic Chemistry, P. Powell, 2<sup>nd</sup> Ed. (ELBS)

## 25032: ORGANIC CHEMISTRY

### UNIT-I: Conformational Analysis

### UNIT-II: Elimination, Esterification & hydrolysis Reactions

### UNIT – III: Addition Reactions

### UNIT-IV: Molecular Rearrangements

#### UNIT-I: Conformational Analysis

15 Hrs

(A) **Conformations of Acyclic Molecules:** Conformations of ethane, propane, n-butane, n-pentane, 2,3-dimethylbutane, 2,3-dibromobutane, butane-2,3-diol, n-propyl chloride, 1,2-dihalogenoethanes, intramolecular hydrogen bonding between two vicinal groups, propionaldehyde, ethylamine, isopropanol, amino alcohol

(B) **Conformations of Cyclic Systems:** Conformations of cyclobutane, cyclopentane, cyclohexane, mono and disubstituted cyclohexanes, cyclohexene, cyclohexanone, 2-alkyl and 3-alkylketone effect, alkylidene cyclohexanes, cycloheptane, decalins, 9-methyldecalin, decalones, decanols

(C) **Conformations of Heterocycles:** Conformations of aziridines, piperidine, 1,3-dioxanes

#### UNIT-II: Elimination, Esterification & hydrolysis Reactions

15 Hrs

(A) **Elimination Reactions:** Type of elimination reactions, mechanisms, Stereochemistry and Orientation, Hofmann and Saytzeff rules, Syn elimination versus anti-elimination, competition between elimination and substitution, dehydration, dehydrogenation, dehalogenation, decarboxylative eliminations, pyrolytic eliminations, molecular rearrangement during elimination, Fragmentation reactions.

(B) **Esterification and hydrolysis:** Mechanism of hydrolysis of Esters, amides and acylhalides, Esterification of acids and transesterification

#### UNIT – III: Addition Reactions

15 Hrs

(A) **Addition to Carbon – Carbon Multiple Bonds:** Mechanistic and stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, region and chemo selectivity, orientation and reactivity, Hydrogenation of double and triple bonds, hydrogenation of aromatic rings, Hydroboration, Sharpless asymmetric epoxidation.

(B) **Addition to Carbon-Hetero Multiple Bonds:** Steric course of addition reactions to C=O and C=N, Cram's rule, Aldol, Cannizzaro, Perkin, Knoevenagel, Claisen-Schmidt, Claisen, Dieckman, Benzoin and Stobbe condensations, Wittig, Grignard, Mannich, and Michael reaction, Hydrolysis of Carbon-Nitrogen bond, Isocyanates and isothioyanates.

#### UNIT-IV: Molecular Rearrangements

15 Hrs

Types of molecular rearrangements, migratory aptitude, Rearrangements to electron deficient carbon: Pinacol-pinacolone, Wagner-Meerwein, Demjanov Arndt-Eistert synthesis and Benzil-Benzilic acid rearrangements; Rearrangements to electron deficient nitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements; Rearrangements to electron deficient oxygen: Baeyer-villiger and Dakin rearrangements; Rearrangements to electron rich carbon: Favorskii and Neber rearrangements

#### Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6<sup>th</sup> Ed. (John Wiley & Sons).
2. Modern Organic Reactions, H. O. House (Benjamin)
3. Structure and Mechanism in Organic Chemistry C. K. Ingold (Cornell University Press).
4. Organic Chemistry, Paula Yurkanis Bruice, 4<sup>th</sup> Ed. (Printice Hall)
5. Organic chemistry-Clayden J. (Oxford)
6. Organic Chemistry, Wade, L.G. Jr. 5<sup>th</sup> Ed. (Pearson)

7. Organic Chemistry, Salmons, P.W. & Others, 8<sup>th</sup> Ed. (John Wiley & Sons)
8. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2<sup>nd</sup> Ed. (Pearson)
9. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.).
10. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6<sup>th</sup> Ed., (Longman).
11. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2<sup>nd</sup> Ed. (New Age International).
12. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
13. Stereochemistry to Organic Compounds, D. Nasipuri, 2<sup>nd</sup> Ed. (New Age International).
14. Stereochemistry, P.S. Kalsi, 5<sup>th</sup> Ed. (New Age International).
15. Organic Chemistry Structure and Reactivity, Ege Seyhan, 3rd Ed. (AITBS)

## 25033: PHYSICAL CHEMISTRY

### UNIT – I: Quantum Chemistry-II

### UNIT – II: Chemical Dynamics –II

### UNIT – III: Thermodynamics-II

### UNIT – IV: Electrochemistry-II

#### UNIT – I: Quantum Chemistry-II

15 Hrs

(A) **Angular momentum:** Angular momentum, Rotations and angular momentum, Eigen functions and Eigen values of angular momentum, Ladder operator, addition of angular momenta, Spin angular momenta, antisymmetry and Pauli Exclusion Principle, Slater determinant,

(B) **Molecular Orbital Theory:** Atomic Orbitals, Simple Molecular Orbitals, Hybrid Atomic Orbitals, Shapes and energies of Molecular Orbital Systems of Organic Molecules (Ex: Methane, Acetylene, ethylene, cyanide anion), Hückel theory of conjugated systems,  $\pi$ -bond order and charge density calculations, application to ethylene, butadiene and benzene.

#### UNIT – II: Chemical Dynamics -II

15 Hrs

(A) **Acid base catalysis: Specific acid catalysis:** General acid catalysis (Hydrolysis of ester and vinyl ether). Specific base catalysis and general base catalysis (the alcohol reaction and hydrolysis of acetic anhydride). Protolytic and prototropic mechanism.

(B) **Homogeneous and Heterogeneous catalysis:** Homogeneous catalysis. Catalysis by transition metal ions and their complexes. Industrially important processes. Supported transition metal complexes as catalysts. Bimolecular reactions. Electronic theories of chemisorption and heterogeneous catalysis.

(C) **Introduction to enzyme catalysis:** Michaelis - Menton Kinetics - Effect of pH and effect of temperature on the rates of enzyme reactions.

#### UNIT – III: Thermodynamics-II

15 Hrs

(A) **Phase Equilibria:** Equilibrium between two phases of one component. The Clapeyron equation. The Clausius Clapeyron equation. Applications. Integrated form of Clapeyron equation.

(B) **Phase rule:** Thermodynamic derivation of phase rule, Solid-liquid equilibria, Thermal analysis, simple eutectic, congruent fusion, incongruent fusion and systems consisting of both. Application of phase rule to three component system, Stokes and Roozeboom plots. Three component liquid systems, formation of one pair, two pairs and three pairs of partially miscible liquids, two salts and water, no chemical combination, double salt formation, one salt forms hydrate and two salts form hydrates, solid solutions.

#### UNIT – IV: Electrochemistry-II

15 Hrs

(A) **Irreversible Electrode Phenomenon:** Reversibility and irreversibility, Dissolution and deposition potentials, Decomposition voltage, overvoltage, diffusion overvoltage, charge transfer overvoltage, reaction overvoltage, concentration overvoltage and phase overvoltage and hydrogen and oxygen over voltages, Tafel plots, Exchange current density and Transfer coefficient, Butler-Volmer equation for one electron transfer processes.

(B) **Deposition and corrosion of metals:** Physical nature of electrodeposited metals – (1) Current density, (2) Concentration of electrolyte, (3) Temperature, (4) Colloidal matter, (5) Electrolyte, (6) Basis metal., throwing power separation of metals by electrolysis, electrochemical passivity, theories of passivity, corrosion of metals, hydrogen evolution type.

### Books Suggested

1. Physical Chemistry, P. W. Atkins, (ELBS)
2. Introduction to quantum Chemistry, A. K. Chandra (Tata McGraw Hill)
3. Quantum Chemistry, Ira N. Levine, (prenticxe Hall)
4. Coulson's Valence, R. Mcweeny, (ELBS)
5. Modern Electrochemistry, vol.I & II, J. O. M. Bockris and A. K. N. Reddy (Plenum)
6. An Introduction to Electrochemistry (3<sup>rd</sup> ed.), S. Glasstone (Affiliated East-West)
7. Micelles, theoretical and applied aspects, V. Moroi (Plenum)
8. A text Book of Physical Chemistry (2<sup>nd</sup> Ed.), S. Glasstone (Macmilan)
9. Principles of Physical Chemistry, Maron and Prutton
10. Theoretical Electrochemistry, L. I. Antropov.

## 25034: GENERAL CHEMISTRY – II

### UNIT – I: X-Ray Diffraction, ORD and CD

### UNIT-II: Separation and Purification Techniques

### UNIT-III: Chromatography

### UNIT-IV: Electro analytical and Thermal techniques

#### UNIT – I: X-Ray Diffraction, ORD and CD

15 Hrs

(A) **X-ray Diffraction:** Bragg conditions, Miller Indices, Laue method, Bragg method, Description of procedure for Debye Scherrer method of X-ray structural analysis of crystals, Index reflections, identification of unit cells from systematic absences in diffraction pattern-structure of simple lattices and X-ray intensities-structure factor and its relation to intensity and electron density.

(B) **Optical Rotatory Dispersion and Circular Dichroism:** Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Axial haloketone rule and octant rule-Application of these rules in the determination of absolute configuration of cyclohexanones and decalones.

#### UNIT-II: Separation and Purification Techniques

15 Hrs

##### (A) Solvent Extraction

Liquid-liquid extraction, Distribution ratio, Factors favouring solvent extraction, Ion-association complexes, Solvent extraction equilibria, Relationship between D and formula of the complex extracted, Separation of actinides using solvent extraction, Super critical fluid extraction.

##### (B) Distillation, Sublimation and Crystallization

Fractional and molecular distillation, Normal and vacuum sublimation, Zone refining, Fractional crystallization.

##### (C) Barrier and Field Separation Methods

Membrane separation: Ultrafiltration; Electro osmosis; Reverse osmosis, Electrophoresis, Ultracentrifugation.

#### UNIT-III: Chromatography

15 Hrs

Definition, classification, Partition or distribution coefficient, Partition ratio, Efficiency, Resolution, Plate height, Plate number, Plate theory, Rate theory, Peak or band asymmetry, Band broadening, Development of Chromatogram, Qualitative and Quantitative applications of chromatography. Principle, process, materials and applications of Paper Chromatography (PC), Thin Layer Chromatography (TLC), Column Chromatography (CC), Size exclusion Chromatography (SEC), Affinity Chromatography, Bonded phase Chromatography, Ion Exchange Chromatography (IEC). High Performance Liquid Chromatography (HPLC): Principle, Instrumentation, pumps, columns, Detectors and Applications of HPLC. Gas Chromatography (GC): Principle, Instrumentation, columns, Detectors and Applications of GC. Super Critical Fluid Chromatography (SFC): Principle, Instrumentation, Applications of SFC.

#### UNIT-IV: Electro analytical and Thermal techniques

15 Hrs

(A) **Electro analytical techniques:** Theory of Potentiometry, types of potentiometric titrations, types of electrodes and their functions, Nernstian response, sources of error in the measurement of potential, Conductometric titrations, Verification of Onsagar equation, calculation of dissociation constant and cell constant, Polarography as an analytical tool for qualitative and quantitative analysis, measurement of diffusion current, Amperometric titrations, Biamperometric titrations, Coulometry at controlled potential and at constant current, HMDE, Anodic stripping voltametry, chronoamperometry and cyclic voltametry.

(B) **Thermal techniques:** TGA and DTA, Interpretation of themogravimetric data, Factors affecting thermal data, Instrumentation and applications.

## Books Suggested

1. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
2. Stereochemistry to Organic Compounds, D. Nasipuri, 2<sup>nd</sup> Ed. (New Age International).
3. Stereochemistry, P.S. Kalsi, 5<sup>th</sup> Ed. (New Age International).
4. Solvent Extraction in Analytical Chemistry, G. H. Morrison and H. Freiser (John Wiley & Sons Inc).
5. Physical and Chemical Methods of Separation, E. W. Berg (McGraw Hill).
6. Separation Process Principles, J. D. Seader and E. J. Henley (John Wiley & Sons Inc).
7. Instrumental Methods of Analysis, H. W. Willard, L. L. Merritt and J. A. Dean (Affiliated East-West)
8. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, 4<sup>th</sup> & 6<sup>th</sup> Ed. (Pearson Education Asia).
9. Principles of Instrumental Analysis, D. A. Skoog and D. M. West (Holt, Rinehart and Wilson)
10. Analytical Chemistry, J. G. Dick (McGraw Hill)
11. Potentiometric Water Analysis, D. Midgley and K. Torrance (John Wiley)



## Laboratory Course (Maximum Marks – 200 Marks)

### II SEMESTER

#### 25031 P: ORGANIC CHEMISTRY PRACTICALS (Marks: 60, Duration: 6 h)

Systematic qualitative analysis of an organic mixture containing two compounds (Identification of method of separation and the functional group (s) present in each of them and preparation of one solid derivative for the conformation of each of the functional group (s))

#### 25032 P: PHYSICAL CHEMISTRY PRACTICALS (Marks: 70, Duration: 6 h)

- (1) Determination of critical solution temperature of phenol-water system and study the effect of electrolyte on CST.
- (2) Determination of eutectic composition and temperature of simple eutectic system (Urea-benzoic acid).
- (3) Determination of congruent composition and temperature of binary system (diphenylamine – benzophenone system)
- (4) Determination of rate constant of acid hydrolysis of an ester and investigate the effect of catalyst concentration, reactant concentration and temperature.
- (5) Conductometry.
  - (a) Determination of cell constant
  - (b) Verification of Onsager equation
  - (c) Determination of dissociation constant of a weak acid
  - (d) Titration of a strong acid with a strong base
  - (e) Titration of a weak acid with a strong base
- (6) Potentiometry
  - (a) Titration of a strong acid with a strong base
  - (b) Titration of a weak acid with a strong base
  - (d) Titration of ferrous ammonium sulphate with potassium dichromate.
- (7) Nuclear techniques
  - (a) Geiger Muller Counter
  - (b) Gamma Ray Spectrometer

#### Books Suggested

1. Adapted from *Introduction to Organic Laboratory Techniques: A Microscale Approach*. Pavia, Lampman, Kriz, and Engel. (1999) Saunders College Publishing.
2. Text book of practical organic chemistry including qualitative organic analysis by A.I. Vogel (Longman)
3. Findlay's Practical Physical Chemistry by J.A. Kitchener, 8<sup>th</sup> Ed. (Longmans)

**THIRD SEMESTER**  
**35031: INORGANIC CHEMISTRY**

**UNIT-I: Spectrophotometry, Flame Photometry and Atomic Absorption Spectroscopy**

**(A) Spectrophotometry**

Beer-lambert law, Photometric accuracy, Deviations from Beer-lambert law, Block-diagram of a spectrophotometer, simultaneous spectrophotometric determination of metals, Determination of ratio of metal complexes: Job's method of continuous variation, slope ratio methods.

**(B) Flame photometry**

Theory and instrumentation, Interferences, background correction, applications.

**(C) Atomic Absorption Spectroscopy**

Theory and instrumentation, Sources of radiation (HCL and EDL), Interferences, background correction, applications.

**UNIT-II: Bioinorganic Chemistry**

**15 Hrs**

**(A) Transport and storage of dioxygen:**

Metal complexes as oxygen carriers, heme proteins – structure and functions of hemoglobin and myoglobin, non-heme proteins – hemoerythrin and hemocyanin, model synthetic complexes of iron, cobalt and copper.

**(B) Electron transfer in biology:**

Structure and functions of metalloproteins in electron transfer process, catalase, peroxidase, cytochromes and iron-sulfur proteins, synthetic models.

**UNIT-III: Photoelectron spectroscopy**

**15Hrs**

Photoelectric effect – Koopmans theorem ionization energy, block diagram of photoelectron spectrometer: sources of radiation, monochromator, detectors, shake-up and shake-off features. Ultraviolet photoelectron spectroscopy, application of UPS to O<sub>2</sub> and N<sub>2</sub> molecules, X-ray photoelectron spectroscopy (ESCA), Applications of XPS to qualitative analysis-chemical shift-application to surface studies and structural analysis.

**UNIT-IV: Introduction to Nanomaterials**

**15Hrs**

Basic chemistry for nanoscience, chemical routes for synthesis of nanomaterials: chemical precipitation and coprecipitation, metal nanocrystals by reduction, sol-gel synthesis, microemulsions or reverse micelles, solvothermal synthesis, microwave heating synthesis, sonochemical synthesis, characterization of nanomaterials: X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM).

**Books Suggested**

1. Instrumental methods of analysis, H. W. Willard, L. L. Merritt and J. A. Dean.
2. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, M. Bochmann and R. N. Grimes, 5<sup>th</sup> Ed. (John Wiley & Sons Inc.).
3. Inorganic Chemistry: Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4<sup>th</sup> Ed (Prentice Hall).
4. Inorganic Chemistry: G. Wulfsberg (University Science Books).
5. Concise Inorganic Chemistry, J. D. Lee, 5<sup>th</sup> Ed. (Wiley-Blackwell).
6. Modern Inorganic Chemistry, W. L. Jolly, 2<sup>nd</sup> Ed. (McGraw-Hill).
7. Introduction to Photoelectron Spectroscopy, P. K. Ghosh
8. Nanochemistry: A Chemical Approach to Nanomaterials; G.A. Ozin, A.C. Arsenault and L. Cademartiri (RSC, London).
9. Nanocomposite Science and Technology; P.M. Ajayan, L.Z. Schadler and P.V. Brown (Wiley).
10. Characterization of Nanophase Materials; Z.L. Wang (ed.) (Wiley-VCH).

## 35032: ORGANIC CHEMISTRY

### UNIT-I: Green Chemistry

15 Hrs

Concept of green chemistry, principles of green chemistry and green synthetic methods – organic reactions in aqueous media: Advantages and applications in Pinacol coupling, Mukaiyama aldol reaction, and Trost-Tsuji reaction; Ionic liquids in organic synthesis: Introduction, composition, and application in stereoselective halogenation, Friedel-Craft reaction and hydroformylation; Microwave assisted reactions: Principle, conditions, advantages over conventional heating methods, and application in Fisher-Indole synthesis, Paal-Knorr pyrrole synthesis, Balis-Hillman and Benzil-Benzilic acid rearrangement; Phase transfer reactions: Introduction, types of phase transfer catalysts, mechanism of catalytic action, and application in Benzoin condensation, Wittig, Wittig-Horner and Michael addition reactions.

### UNIT – II: Photochemistry

15 Hrs

Photochemical energy, Frank Condon principles, Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency and quantum yield. Photochemistry of carbonyl compounds:  $n \rightarrow \pi^*$  and  $\pi \rightarrow \pi^*$  transitions, Norrish type I and Norrish type- II cleavages, Paterno-Buchi reactions, Photo reduction, Rearrangement of cyclohexenones, cyclohexadienones. Photochemistry of unsaturated systems (olefins): *Cis-trans* isomerization, photochemistry of 1,3-butadienes, Di- $\pi$ -methane rearrangement, Oxa-di- $\pi$ -methane rearrangement. Photochemistry of aromatic compounds: Photoisomerization of aromatic compounds, photo Fries rearrangement, photo Fries reactions of anilides. Photolysis of nitric esters and Barton reaction.

### UNIT-III: Pericyclic reactions

15 Hrs

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system and 2,4-pentadienyl systems, classification of pericyclic reactions, Electrocyclic reactions: Conrotatory and Disrotatory motions in  $4n$ ,  $4n+2$  systems, FMO and PMO approach, Woodward-Hoffmann Correlation diagrams and Woodward-Hoffmann selection rules of electrocyclic reactions. Cycloadditions: antarafacial and suprafacial additions in  $4n$  ( $2+2$  cyclo addition) and  $4n+2$  ( $4+2$  cyclo addition) systems, FMO and PMO approach, Woodward-Hoffmann Correlation diagrams and Woodward-Hoffmann selection rules of cyclo addition reactions,  $2+2$  addition of ketene, 1,3-dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements – 1,3 and 1,5 suprafacial and antarafacial shifts of H and C, FMO and PMO approach and Woodward-Hoffmann selection rules of sigmatropic rearrangements, Claisen, Cope and oxy-Cope rearrangements, Ene reaction.

### UNIT-IV: Asymmetric synthesis

15 Hrs

#### (A) Introduction and terminology

Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic), Prochirality nomenclature; Substitution and addition criteria. Pro-R, Pro-S, Re and Si faces. Stereoselective reactions: Enantioselectivity and diastereoselectivity. Optical purity: Enantiomeric excess and diastereomeric excess.

#### (B) Strategies in Asymmetric Synthesis

**i. Chiral substrate controlled asymmetric synthesis:** Nucleophilic additions to chiral carbonyl compounds. 1, 2-asymmetric induction, Cram's rule and Felkin-Anh model.

**ii. Chiral auxiliary controlled asymmetric synthesis:**  $\alpha$ -Alkylation of chiral enolates, azaenolates, imines. Use of chiral auxiliaries in Diels-Alder reaction and Aldol reactions

**iii. Chiral reagent controlled asymmetric synthesis:** Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2 BH and IPCBH2.

**iv. Chiral catalyst controlled asymmetric synthesis:** Sharpless and Jacobsen asymmetric epoxidations. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalyst. Enzyme mediated enantioselective synthesis.

#### Books Suggested:

1. Green Chemistry: an introductory text; M. Lancaster; 2<sup>nd</sup> Ed. (RSC).
2. Organic Synthesis: Special Techniques; V.K. Ahluwalia and R. Aggarwal; 2<sup>nd</sup> Ed. (Narosa)

3. Fundamentals of Photochemistry, K. K. Raotagi-Mukhergi, (Wiley Eastern)
4. Essential of Molecular Photochemistry, A. Gilbert and J. Baggott (Blackwell scientific Publications)
5. Organic Photochemistry, J. Coxon and B. Halton, (Cambridge University Press)
6. Pericyclic Reactions, S. M. Mukheriji, (Macmillan)
7. Stereochemistry to organic Compounds, D. Nasipuri, 2<sup>nd</sup> Ed. (New Age International).
8. Advanced Organic Chemistry, Part B: reactions and syntesis; F.A. Carey and R.J. Sundberg; 5<sup>th</sup> Ed. (Springer Verlag).
9. Asymmetric synthesis by Nogradi
10. Asymmetric organic reactions by J D Morrison and H S Moschr
11. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey Aube

## 35033: PHYSICAL CHEMISTRY

### UNIT – I: Surface Chemistry

15 Hrs

Structural and theoretical treatment of liquid interfaces, thermodynamics of binary system, Gibbs equation and verification of Gibbs equation by microtome method and tracer method, spreading of one liquid on another, states of monomolecular films, the surface area of solids, mixed films, Gibbs adsorption isotherm, the Langmuir adsorption isotherm, BET adsorption isotherm, estimation of surface area (BET equation, theoretical concept), adsorption time. Non equilibrium thermodynamics (entropy production in irreversible process), membrane transport in biochemical reactions.

### UNIT – II: Polymers-Basics and Characterization

15 Hrs

#### (A) Basic concepts

Monomers, repeat units, degree of polymerization, linear, branched and network polymers, classification of polymers.

#### (B) Polymerization methods

Condensation, addition, radical chain, ionic and coordination, copolymerization, controlled free radical polymerisation (viz. ATRP, RAFT and NMP).

#### (C) Average molecular weight concepts

Number, weight and viscosity average molecular weights, polydispersity and molecular weight distribution, measurement of molecular weight: end group, viscosity, light scattering, osmotic and ultracentrifugation methods.

### UNIT – III: Electro kinetic Phenomena and Batteries

15 Hrs

#### (A) Electro kinetic Phenomena

Electro osmosis, electro phoresis, streaming potential, Influence of ions on electro kinetic phenomena, Sterns Treatment of Electrical Double layer and its structure, Zeta potential

#### (B) Batteries

Batteries Primary and secondary batteries-Fuel cells-Proton exchange membrane fuel cells-Advantage and limitations of fuel cells working principles of UPS and its applications.

### UNIT – IV: Nuclear Techniques

15 Hrs

Basic concepts of nuclear chemistry, radioactive decay and equilibrium, nuclear reactions, Q value, cross sections, types of nuclear reactions; radioactive techniques: counting techniques such as G. M. ionization and proportional counter, isotopic dilution, neutron activation analysis, radiometric titration; radiopharmaceuticals: radioimmunoassay, immunoradiometric assay, classification of radiopharmaceuticals, labeled compounds preparation, PET studies.

#### Books Suggested

1. Physical methods in Chemistry, R. S. Drago (Saunders College).
2. Principles of Physical Chemistry by Samuel H. Maron and Carl F. Prutton. The Mac Millan Company, New York.
3. Advanced Physical Chemistry by GurudeepRaj, Goel Publishers House, Meerut.
4. An introduction to Electrochemistry-4th edn: By Samuel Glasstone Affiliated East West Press Pvt. Ltd., New Delhi.
5. Electrochemistry by M. S. Yadav Anmol Publications, New Delhi.
6. Essentials of Nuclear Chemistry, 4th Ed., 1995, H. J. Harnikar (Wiley Eastern)
7. Electrochemistry by S. Glasstone.
8. Text Book of Polymer Science, F. W. Billmeyer, Jr. (Wiley Inter Science)
9. Polymer Chemistry, Gowarikar.

## 35034: SPECTROSCOPY AND ITS APPLICATIONS

### UNIT-I: UV-Visible and IR Spectroscopy

15 Hrs

#### (A) Ultraviolet and Visible Spectroscopy

Various electronic transitions (185-800 nm), effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes and conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls, polycyclic aromatic compounds.

#### (B) Infrared Spectroscopy

Instrumentation and sample handling, FT-IR. overtones, combination bands and Fermi resonance, factors influencing vibrational frequencies, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds).

### UNIT-II: Nuclear Magnetic Resonance Spectroscopy ( $^1\text{H}$ NMR)

15 Hrs

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, deshielding, chemical shifts and its measurements, factors influencing chemical shift, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines and amides), spin-spin interactions, coupling constant (J): Types and classification (ABX, AMX, ABC etc.) of coupling constants, factors influencing coupling constants, Karplus curve variation of coupling constant with dihedral angle, complex spin-spin interaction between two, three, four and five nuclei (First order spectra), virtual coupling, chemical exchange, effect of deuteration, hindered rotation, Simplification of complex spectra: nuclear magnetic double resonance (spin decoupling), contact shift reagents, Nuclear Overhauser effect (NOE).

### UNIT-III: $^{13}\text{C}$ NMR spectroscopy & 2D NMR techniques

15 Hrs

#### (A) $^{13}\text{C}$ NMR spectroscopy

CW and FT techniques. Types of  $^{13}\text{C}$  NMR spectra: uncoupled, proton- decoupled and offresonance decoupled (ORD) spectra.  $^{13}\text{C}$  chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ( $^{13}\text{C}$ - $^{13}\text{C}$  J) and heteronuclear ( $^{13}\text{C}$ - $^1\text{H}$  J) coupling.  $^{13}\text{C}$ -NMR spectral editing techniques: principle and applications of APT and DEPT methods.

#### (B) 2D NMR techniques

Principles of 2D NMR, classification of 2D-experiments. Correlation spectroscopy (COSY), HOMO COSY ( $^1\text{H}$ - $^1\text{H}$  COSY), COSY of m-dinitrobenzene, isopentyl acetate, Hetero COSY ( $^1\text{H}$ , $^{13}\text{C}$  COSY) Hetero COSY of isopentyl acetate and 4-methyl-2-pentanol, HMQC, HMQC of codeine, long range  $^1\text{H}$ , $^{13}\text{C}$  COSY (HMBC), HMBC of codeine and NOESY, NOESY of 9-benzylanthracene, 2-D INADEQUATE experiments

### UNIT-IV: Mass Spectrometry

15 Hrs

Introduction, Principle, Instrumentation, Single & Double focusing Mass Spectrometers, Ionization Methods: EI, CI, FDI, PDI, LDI, FAB, TSI and ESI, Mass Analyzers: MSA, ESA, QMA, ITA, TOF, FT and Tandem, Molecular-ion peak, Nitrogen rule, Base peak, Metastable ion, isotopic abundance, High resolution mass spectrometry (HRMS), Index of hydrogen deficiency (IHD), General methods of mass spectral fragmentation, Mc. Lafferty rearrangement, Ortho effect, Factors affecting fragmentation, Mass spectral fragmentation patterns of various classes of organic compounds, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

#### Books suggested

1. Organic spectroscopy, W. Kemp, 5<sup>th</sup> Ed., (ELBS.2)
2. Spectroscopy of organic compounds, R.M. Silverstein and others, 5<sup>th</sup> Ed., (John Wiley)
3. Spectrometric Identification of organic compounds, R.M. Silverstein, F.X. Webster and D.J. Kiemle, 7<sup>th</sup> Ed., (Wiley)
4. Introduction to Spectroscopy, A guide for students of organic chemistry, Donald L. Pavia, Gary M. Lamp man and George S. Kriz, 3<sup>rd</sup> Ed., (Thomson).
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemming, (TMH)
6. Spectroscopy of organic compounds, P. S. Kalsi, (Wiley)
7. Nuclear Magnetic Resonance Spectroscopy An introduction to Principles, Applications and experimental methods, Joseph B. Lambert and Eugene P. Mazzola, (Pearson Education Inc. Prentice – Hall).
8. A Complete Introduction to Modern NMR Spectroscopy, Roger S. Macomber, (John Wiley & Sons, Inc.).

## Laboratory Course-200 MARKS

### III – SEMESTER

#### 45031- P: Chromatographic Separation and Isolation & identification of Natural Products

1. Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R<sub>f</sub> values of known standards.
2. Separation by column chromatography: Separation of a mixture of *ortho* and *para* nitroanilines using silicagel as adsorbent and chloroform as the eluent. The column chromatography should be monitored by TLC.
3. Isolation and identification of Natural Products
  - (a) Isolation of caffeine from tea leaves
  - (b) Isolation of eugenol from cloves
  - (c) Isolation of casein and lactose from milk
  - (d) Isolation of limonene from lemon peel
  - (e) Isolation of piperines from black pepper
  - (f) Isolation of lycopene from tomatoes
  - (g) Isolation of β-carotene from carrots

#### 45032-P: Estimations

Estimation of (a) Glucose (b) Phenol (c) Aniline (d) Acetone (e) Aspirin (f) Ibuprofen (g) Paracetamol

**Educational Tour:** A visit to research institutes and pharmaceutical companies as a part of an educational tour.

#### Books Suggested:

1. Ikan, R. *Natural Products, A Laboratory Guide*, 2nd ed.; Academic Press: New York, 1991.
2. Adapted from *Introduction to Organic Laboratory Techniques: A Microscale Approach*. Pavia, Lampman, Kriz, and Engel. (1999) Saunders College Publishing.
3. Pharmaceutical drug analysis by Ashutoshkar
4. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
5. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
6. Practical organic chemistry by Mann & Saunders
7. Text book of practical organic chemistry including qualitative organic analysis by A.I. Vogel (Longman)

**FOURTH SEMESTER**  
**45031: REACTIONS AND REAGENTS IN ORGANIC SYNTHESIS**

**UNIT-I: Oxidations and Reductions**

**15 Hrs**

**(A) Oxidations**

(a) Alcohols to carbonyls: Chromium (vi) Oxidants: Dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, DDQ, oxidation with silver carbonate (b) Alkenes to epoxide: peroxide induced epoxidations (c) Alkenes to diols: oxidation with potassium permanganate, osmium tetroxide, Prevost reaction, Wood-Word modification (d) Ketones to esters: Baeyer-Villiger oxidation (e) Oxidation of alkyl or alkenyl fragments: selenium dioxide.

**(B) Reductions**

a) Nucleophilic metal hydrides:  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , Red-Al and alkoxy aluminates b) Electrophilic metal hydrides:  $\text{BH}_3$ ,  $\text{AlH}_3$  and DIBAL c) Non-metallic reductions: Diimide reduction, Wolf-Kishner Reduction d) Dissolving metal reductions: Birch reduction e) Heterogeneous catalytic hydrogenation.

**UNIT- II: Non-Metallic Reagents in Organic Synthesis**

**15 Hrs**

Electronic structure and bonding in Boron, Phosphorus and Sulphur compounds – Their reactivity and applications in Organic Synthesis.

**(A) Boron Reagents**

Hydroboration, Organoboranes in the formation of C-C bonds, alcohols, amines, halogen and carbonyl compounds, Free radical reactions of Organoboranes.

**(B) Phosphorus Reagents**

Formation of C-C double bonds (Witting reaction, Horner-Wordsworth-Emmons reaction), Functional group transformations, Reactivity as electrophiles and nucleophiles.

**(C) Sulphur Reagents**

Sulphur ylides, stabilised and non-stabilised, Preparation and reactivity, sulphonyl carbanions.

**(D) Silicon reagents**

Reactions involving  $\beta$ -carbocations and  $\alpha$ -carbanions, utility of trimethyl silyl halides, cyanides and triflates

**UNIT-III: Metallic Reagents in Organic Synthesis**

**15Hrs**

**(A) Synthesis and applications organometallic reagents:**

Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium, Rhodium and Nickel reagents in Organic synthesis.

**(B) Metal mediated C-C and C-X coupling reactions:**

Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.

**UNIT-IV: Advanced Synthetic reactions and concepts in organic synthesis**

**15 Hrs**

**(A) C=C Formation Reactions**

Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.

**(B) Multicomponent Reactions**

Ugi, Passerini, Biginelli, Hantzsch and Mannich reactions.

**(C) Ring Formation Reactions**

Pausan-Khand reaction, Bergman cyclisation, Nazarov cyclisation

**(D) Click Chemistry**

Criteria for Click reaction, Sharpless azides cycloadditions.

**(E) Metathesis**

Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.

**(F) Tandem synthesis**

Tandem reactions; conjugate addition-aldol reaction, polymerization- cyclisation, electrocyclic-Diels Alder reaction.

**(G) Baldwin Rules**

Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.



**Books Suggested:**

1. Modern Synthetic Reactions, H. O. House, 2<sup>nd</sup> Ed., (W.A. Benjamin)
2. Modern Methods of Organic Synthesis, W. Carruthers, 3<sup>rd</sup> Ed., (Cambridge University Press).
3. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, (Blakie Academic and Professional).
4. Advanced Organic Chemistry Part A& B, F. A Carey and R. J. Sundberg, 5<sup>th</sup> Ed., (Springer Science + Business Media).
5. Guide book to Organic Synthesis, R. K. Machie and D.N.Smith, (ELBS).
6. Principles of organometallic chemistry, P.Powell, (ELBS).
7. Organo transition metal chemistry-Applications to organic synthesis, S.G.Davis, Pergmon.
8. Multi-component Reactions: J. Zhu and H. Bienaymé (Wiley-VCH).
9. Strategies for organic drug synthesis and design By Daniel Ledneicer.

## 45032: SYNTHETIC STRATEGIES AND DRUG DESIGN

### UNIT-I: Synthetic Strategies -I

15 Hrs

#### (A) Disconnection Approach

Synthetic Strategies; Introduction, Terminology: target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity (umpolung) and cyclizations. Order of events in synthesis by retrosynthetic approach, explanation with examples salbutamol, Propoxycaïne and Dinocap. Introduction to one group C-C and C-X disconnections. One group C-C disconnections, Alcohols and carbonyl compounds. One group C-X disconnections, Carbonyl compounds, alcohols, ethers and sulphides.

#### (B) Protecting Groups

Principles of protection of alcohol, amine, carbonyl and carboxyl groups

### UNIT-II: Synthetic Strategies -II

15 Hrs

#### (A) One Group C-C Disconnections

Alcohols and carbonyl compounds, Regioselectivity, Alkene synthesis, use of acetylenic compounds in organic synthesis.

#### (B) Two Group C-C Disconnections

Diels-Alder reaction, 1,3-difunctionalised Compounds, unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

#### (C) Ring Synthesis

Introduction to ring synthesis, cyclization of saturated heterocycles – three, four, five, six and seven membered ring systems.

#### (D) Disconnections of Target Molecules

i) 3-(cyclohex-3-enyl)propanoic acid, ii) (Z)-hept-5-en-2-one, N-(3,4-dimethoxyphenethyl)-2-(3,4-dimethoxyphenyl)acetamide, iii) 2-(dimethylamino)ethyl-2-(1-hydroxycyclopentyl)-2-phenylacetate, iv) 1-(1-hydroxy-2-phenylethyl)cyclohexanol, v) 5-methyl-6,8-dioxabicyclo[3.2.1]octane, vi) 1-(4-chlorophenyl)-2,5-dimethyl-1H-pyrrole-3-carboxylic acid, vii) 4a-ethyloctahydroquinolin-7(1H)-one, viii) ethyl 2,6-dioxo-1,4-diphenylpiperidine-3-carboxylate, ix) methyl 1,2-dimethyl-4-phenyl-1,4-dihydropyridine-3-carboxylate

### UNIT-III: Principles of Drug design and Development

15 Hrs

#### (A) Basic principles of Pharmacology

Definitions: disease, drug, bioassay, pharmacokinetics and pharmacodynamics. Stages involved in drug discovery. Pharmacokinetics (ADME): Routes of drug administration, Absorption, Distribution, Metabolism and Excretion of drugs. Pharmacodynamics: Nature of drug – receptor interactions, Theories of drug action: Occupancy theory, Rate theory, Induced-fit theory, and Macromolecular perturbation theory. Drug synergism and antagonism, drug toxicity, clinical trials.

#### (B) Drug design

Lead discovery, Existing drugs as leads (me too drugs), Pharmacophore, Principles of design of agonists (e.g. Salbutamol), antagonists (e.g. cimetidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity-Penicillin and Librium as examples.

### UNIT- IV: SAR and QSAR studies

15 Hrs

#### (A) Lead modification strategies

Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxaminquine.

#### (B) Structure-Activity Relationship studies(SAR)

SAR in sulfa drugs, benzodiazepines and taxol analogs. Principles of prodrug design.

#### (C) Quantitative Structure- Activity Relationship (QSAR)

Introduction to QSAR, physicochemical properties – Lipophilicity: partition coefficient (P) and the lipophilicity substituent constant ( $\sigma$ ), Electronic effects: Hammett constants ( $\sigma$ ), Steric effects: Taft's constant ( $E_s$ ), Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, Lipinski rule of five.

**Books Suggested:**

1. Designing Organic Syntheses: A Programmed Introduction to the Synthron Approach, S. Warren, (John Wiley & Sons)
2. Organic Synthesis: Strategy and Control, Paul Wyatt, Stuart Warren, (John Wiley & Sons)
3. Guide book to Organic Synthesis, R.K.Mackie and D.N.Smith, (ELBS)
4. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop and G. Perzillin, (Verlage VCH)
5. Some Modern Methods of Organic Synthesis, W. Carruthers, 3<sup>rd</sup> Ed., (Cambridge Univ. Press).
6. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
7. An Introduction to Medicinal chemistry by Patrick.
8. Medicinal chemistry An introduction by Garreth Thomas

## 45033: HETEROCYCLIC CHEMISTRY AND BIOMOLECULES

### UNIT – I: Nomenclature, Aromaticity Reactivity and Three membered Heterocycles 15 Hrs

#### (A) Nomenclature of Heterocycles

Systematic Nomenclature (Hantzsch-Widman system), trivial system, fusion nomenclature system. Replacement nomenclature system; Monocyclic heterocycles, fused heterocycles, spiro heterocycles. Bridged heterocycles; bicyclic systems, polycyclic systems, Heterocyclic ring assemblies.

#### (B) Aromaticity of Heterocycles

Chemical behaviour of aromatic heterocycles; Five and six-membered aromatic heterocycles and mixed aromatic heterocycles, Relationship with carbocyclic aromatic compounds  
Criteria of aromaticity in heterocycles; Structural and electronic criteria.

#### (C) Hetero aromatic reactivity

Selectivity and reactivity in heteroaromatic rings; Five and six-membered heterocyclic rings.

#### (D) Three membered Heterocycles

Synthesis, chemical reactions of aziridines, oxiranes, oxaziridines, thiiranes

### UNIT–II: Four membered and Five membered (with two heteroatoms) Heterocycles 15 Hrs

#### (A) Four membered Heterocycles

Synthesis, chemical reactions of, azetidines, azetidinones ( $\beta$ -Lactams), oxetanes, oxetanones ( $\beta$ -Lactones) and thietanes.

#### (B) Five membered with two heteroatoms

Synthesis, chemical reactions of pyrazole, imidazole, isoxazole, oxazole, isothiazole and thiazole.

### UNIT –III: Benzofused Five and Six membered Heterocycles 15 Hrs

#### (A) Benzofused Five Membered Heterocycles

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans, bezothiophenes and benzimidazoles.

#### (B) Benzofused Six Membered Heterocycles

Synthesis and reactions including medicinal applications of quinoline and Isoquinoline

### UNIT–IV: Biomolecules 15 Hrs

#### (A) Enzymes

Definition. Classification based on mode of action. Mechanism of enzyme catalysis. Factors affecting enzyme catalysis. Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis.

(B) Nucleic acids: Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA.

Replication, transcription and translation. Genetic code. Chemical Synthesis of nucleosides and nucleotides.

#### Books Suggested:

1. Heterocyclic Chemistry Vol.1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Verlag
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme
3. Heterocyclic Chemistry, J.A.Joule, K. Killis and G. F. Smith, Chapman and Hall
4. Heterocyclic Chemistry, T.L.Gilchrist, Longman Scientific Technical
5. Heterocyclic Chemistry, Raj.K. Bansal.
6. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, eds., Pergamon Press
8. Principles of Modern Heterocyclic Chemistry, L. A. Paquett.
9. Enzyme structure and mechanism by Fersht and Freeman.
10. Bio-Organic chemistry by Hengan Dugas
11. Nucleic acids in Chemistry and Biology by G M Blackburn MI Gait
12. Lehninger Principles of Biochemistry by D L Nelson and M M Cox.

## 45034: CHEMISTRY OF NATURAL PRODUCTS

### UNIT-I: Terpenoids

15 Hrs

Occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of Camphor, Farnesol, Zingiberene, Cadinene, Abietic acid and Lanosterol.

### UNIT-II: Alkaloids

15 Hrs

Introduction, isolation, general methods of structure elucidation and physiological action, degradation, classification based on nitrogen heterocyclic ring, structure, stereochemistry, synthesis and biosynthesis of morphine, strychnine and reserpine

### UNIT-III: Steroids and Prostaglandins

15 Hrs

#### (A) Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and its stereochemistry. Isolation, structure determination and synthesis of cholesterol (total synthesis not expected), androsterone, testosterone, estrone and progesterone, Biosynthesis of steroids.

#### (B) Prostaglandins

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE<sub>2</sub> and PGF<sub>2</sub>

### UNIT-IV: Flavonoids and Isoflavonoids

15 Hrs

Occurrence, nomenclature and general methods of structure determination, Isolation, structure elucidation and synthesis of apigenin, luteolin, kaempferol, quercetin, butein, daidzein. Biosynthesis of flavonoids and Isoflavonoids: Acetate Pathway and Shikimic acid Pathway.

### Books Suggested

1. Natural Products: Chemistry and Biological Significance, J. Mann, R.S.Davidson, J. B. Hobbs, D. V. Banthrope and J. B. Hatrbnome, Longman, Essex.
2. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
3. Chemistry of Organic Natural Products, O. P. Agrawal, Vols. 1 &2, Goel Pubs.
4. Natural Products Chemistry K. B. G. torssell, John Wiley, 1983
5. New Trends in Natural Products Chemistry, Atta-ur-Rahman and M.I.Choudhary, Harwood Academic Publisher.
6. Chemistry of Natural products P. S. Kalsi, Kalyani Publishers
7. Biosynthesis of steroids, terpenes and acetogenins, J. H. Richards & J. R. Hendrieson
8. The biosynthesis of secondary metabolites, R. D. Herbert, Chapman & Hall
9. The Biosynthesis of Secondary Metabolite, R. D. Herbert, Second edn, Chapman and Hall 1984

## Laboratory Course-200 MARKS

### IV-SEMESTER

#### 45031- P : Multistep Synthesis of Organic Compounds:

The experiments should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

1. Beckmann rearrangement: Benzanilide from Benzophenone  
Benzophenone → Benzophenone oxime → Benzanilide
2. Benzilic acid rearrangement: Benzilic acid from benzoin  
Benzoin → Benzil → Benzilic acid
3. P-Bromo Aniline from Aniline :  
Aniline → Acetanilide → P-Bromo Acetanilide → P-Bromo Aniline
4. Symmetrical Tribromo Benzene from aniline:  
Aniline → Tribromoaniline → Tribromobenzene
5. 2,4,6-trimethylquinoline from p-toluidine  
p-toluidine → 4-(p-tolylamino)pent-3-ene-2-one → 2,4,6-trimethylquinoline
6. Flavone from o-hydroxy acetophenone  
o-hydroxy acetophenone → o-benzoyl acetophenone → o-hydroxy- dibenzoylmethane → Flavone
7. 2-phenylindole from phenylhydrazine  
phenylhydrazine → acetophenone phenylhydrazone → 2-phenylindole

#### 45032-P : Spectral Identification of Organic Compounds (UV, IR, <sup>1</sup>H- and <sup>13</sup>C- NMR, MASS).

A minimum of 40 representative examples should be studied

#### Books Suggested

1. Modern Organic Synthesis in the Laboratory *A Collection of Standard Experimental Procedures*  
Jie Jack Li, Chris Limberakis, Derek A. Pflum
2. Practical organic chemistry by Mann & Saunders
3. Text book of practical organic chemistry by Vogel
4. Spectrometric Identification of organic compounds, R.M. Silverstein, F.X. Webster and D.J. Kiemle, 7<sup>th</sup> Ed.,  
(Wiley)